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C13 0.0219(16) 0.0204(15) 0.0297(17) 0.0021(12) 0.0116(13) 0.0038(12)
C14 0.0195(16) 0.0239(16) 0.0302(17) 0.0032(13) 0.0038(13) 0.0106(13)
C15 0.0184(15) 0.0164(14) 0.0172(14) 0.0059(11) 0.0038(12) 0.0041(11)
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C17 0.0341(18) 0.0145(14) 0.0201(15) 0.0058(11) 0.0086(13) 0.0051(13)
C18 0.072(3) 0.0174(16) 0.0260(18) 0.0025(14) 0.0037(18) -0.0054(17)
C19 0.042(2) 0.0198(15) 0.0287(17) 0.0104(13) 0.0118(15) 0.0050(14)
C20 0.055(2) 0.0329(18) 0.0356(19) 0.0209(15) 0.0265(17) 0.0304(17)
C21 0.0157(14) 0.0136(13) 0.0197(14) 0.0001(11) 0.0051(12) 0.0033(11)
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C24 0.0222(16) 0.0179(14) 0.0224(15) -0.0041(12) 0.0065(13) 0.0045(12)
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C27 0.0230(16) 0.0244(15) 0.0189(15) 0.0089(12) 0.0062(12) 0.0131(13)
C28 0.0387(19) 0.0231(16) 0.0287(17) 0.0139(13) 0.0186(15) 0.0131(14)
C29 0.0205(15) 0.0211(15) 0.0232(15) 0.0114(12) 0.0104(12) 0.0098(12)
C30 0.0208(16) 0.0245(16) 0.0436(19) 0.0102(14) 0.0128(15) 0.0091(13)
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C43 0.055(5) 0.028(4) 0.023(4) 0.008(3) 0.016(3) 0.027(4)
C44 0.034(4) 0.018(3) 0.039(4) 0.005(3) 0.010(3) 0.007(3)
C45 0.028(4) 0.039(5) 0.023(4) 0.002(3) 0.002(3) 0.004(4)
C46 0.053(5) 0.026(3) 0.033(4) 0.009(3) 0.014(4) 0.016(3)
C47 0.023(4) 0.037(4) 0.037(4) 0.010(3) 0.012(3) 0.012(3)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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C41 C46 1.266(10) 2_556 ?
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_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'Bruker SHELXTL'
_computing_publication_material   'Bruker SHELXTL'

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and
is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F, and
R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            'Full matrix'
_refine_ls_weighting_scheme       Sigma
_refine_ls_weighting_details      'w=1/s^2^(Fo^2^)'
_atom_sites_solution_primary      'Direct methods'
_atom_sites_solution_secondary    'Difference Fourier map'
_atom_sites_solution_hydrogens    'Geometric positions'
_refine_ls_hydrogen_treatment     Riding
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details
 'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack    -0.08(3)
_refine_ls_number_reflns          16726
_refine_ls_number_parameters      765
_refine_ls_number_restraints      1
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_refine_ls_R_factor_gt            0.0374
_refine_ls_wR_factor_ref          0.0643
_refine_ls_wR_factor_gt           0.0604
_refine_ls_goodness_of_fit_ref    1.130
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Zr1 Zr 0.46482(3) 0.991292(17) 0.39171(3) 0.01140(10) Uani 1 1 d . . .
Cl1A Cl 0.50015(9) 1.11077(6) 0.36243(8) 0.0174(3) Uani 1 1 d . . .
Cl2A Cl 0.30897(9) 0.99935(6) 0.44558(7) 0.0173(2) Uani 1 1 d . . .
Si1A Si 0.65576(10) 0.92432(7) 0.32878(8) 0.0133(3) Uani 1 1 d . . .
Si2A Si 0.48238(11) 0.82699(7) 0.41337(9) 0.0135(3) Uani 1 1 d . . .
C1A C 0.6376(3) 0.9368(2) 0.4492(3) 0.0134(11) Uani 1 1 d . . .
C2A C 0.5647(4) 0.8978(3) 0.4850(3) 0.0158(11) Uani 1 1 d . . .
C3A C 0.5406(3) 0.9398(2) 0.5554(3) 0.0135(11) Uani 1 1 d . . .
H3A H 0.4942 0.9269 0.5907 0.016 Uiso 1 1 calc R . .
C4A C 0.5956(3) 1.0036(3) 0.5651(3) 0.0127(11) Uani 1 1 d . . .
C5A C 0.6534(3) 1.0001(3) 0.4981(3) 0.0140(10) Uani 1 1 d . . .
H5A H 0.6973 1.0361 0.4876 0.017 Uiso 1 1 calc R . .
C6A C 0.5090(3) 0.9254(2) 0.2698(3) 0.0141(11) Uani 1 1 d . . .
C7A C 0.4356(4) 0.8834(2) 0.3050(3) 0.0139(10) Uani 1 1 d . . .
C8A C 0.3322(3) 0.9139(3) 0.2670(3) 0.0140(10) Uani 1 1 d . . .
C9A C 0.3447(4) 0.9729(2) 0.2153(3) 0.0128(11) Uani 1 1 d . . .
H9A H 0.2898 1.0044 0.1867 0.015 Uiso 1 1 calc R . .
C10A C 0.4485(3) 0.9788(2) 0.2118(3) 0.0125(10) Uani 1 1 d . . .
C11A C 0.7265(4) 1.0012(3) 0.3038(3) 0.0212(12) Uani 1 1 d . . .
H11A H 0.7995 1.0005 0.3449 0.032 Uiso 1 1 calc R . .
H11B H 0.6914 1.0431 0.3159 0.032 Uiso 1 1 calc R . .
H11C H 0.7260 1.0004 0.2373 0.032 Uiso 1 1 calc R . .
C12A C 0.7277(4) 0.8472(3) 0.3097(3) 0.0204(12) Uani 1 1 d . . .
H12A H 0.7768 0.8600 0.2744 0.031 Uiso 1 1 calc R . .
H12B H 0.6775 0.8129 0.2735 0.031 Uiso 1 1 calc R . .
H12C H 0.7671 0.8276 0.3711 0.031 Uiso 1 1 calc R . .
C13A C 0.5582(4) 0.7484(3) 0.4006(3) 0.0221(12) Uani 1 1 d . . .
H13A H 0.5404 0.7104 0.4369 0.033 Uiso 1 1 calc R . .
H13B H 0.6339 0.7581 0.4247 0.033 Uiso 1 1 calc R . .
H13C H 0.5402 0.7355 0.3336 0.033 Uiso 1 1 calc R . .
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C14A C 0.3759(3) 0.8005(2) 0.4648(3) 0.0176(10) Uani 1 1 d . . .
H14A H 0.4064 0.7738 0.5229 0.026 Uiso 1 1 calc R . .
H14B H 0.3242 0.7720 0.4189 0.026 Uiso 1 1 calc R . .
H14C H 0.3410 0.8416 0.4797 0.026 Uiso 1 1 calc R . .
C15A C 0.5947(3) 1.0615(3) 0.6308(3) 0.0166(11) Uani 1 1 d . . .
H15A H 0.5968 1.1049 0.5949 0.020 Uiso 1 1 calc R . .
C16A C 0.4927(3) 1.06363(18) 0.6583(3) 0.0217(8) Uani 1 1 d . . .
H16A H 0.4324 1.0657 0.6009 0.033 Uiso 1 1 calc R . .
H16B H 0.4926 1.1045 0.6973 0.033 Uiso 1 1 calc R . .
H16C H 0.4875 1.0220 0.6945 0.033 Uiso 1 1 calc R . .
C17A C 0.6957(3) 1.0624(2) 0.7201(3) 0.0186(9) Uani 1 1 d . . .
C18A C 0.7953(3) 1.0687(2) 0.6899(3) 0.0352(11) Uani 1 1 d . . .
H18A H 0.7905 1.1096 0.6498 0.053 Uiso 1 1 calc R . .
H18B H 0.8032 1.0274 0.6541 0.053 Uiso 1 1 calc R . .
H18C H 0.8566 1.0730 0.7462 0.053 Uiso 1 1 calc R . .
C19A C 0.6898(3) 1.1263(2) 0.7824(3) 0.0280(11) Uani 1 1 d . . .
H19A H 0.7566 1.1312 0.8329 0.042 Uiso 1 1 calc R . .
H19B H 0.6322 1.1201 0.8105 0.042 Uiso 1 1 calc R . .
H19C H 0.6770 1.1679 0.7429 0.042 Uiso 1 1 calc R . .
C20A C 0.7021(3) 0.9989(2) 0.7805(3) 0.0328(10) Uani 1 1 d . . .
H20A H 0.7649 1.0016 0.8356 0.049 Uiso 1 1 calc R . .
H20B H 0.7065 0.9578 0.7431 0.049 Uiso 1 1 calc R . .
H20C H 0.6391 0.9959 0.8019 0.049 Uiso 1 1 calc R . .
C21A C 0.2283(4) 0.8847(2) 0.2690(3) 0.0138(10) Uani 1 1 d . . .
H21A H 0.2323 0.8748 0.3364 0.017 Uiso 1 1 calc R . .
C22A C 0.2090(3) 0.8162(2) 0.2139(3) 0.0184(10) Uani 1 1 d . . .
H22A H 0.2095 0.8247 0.1480 0.022 Uiso 1 1 calc R . .
H22B H 0.2671 0.7839 0.2434 0.022 Uiso 1 1 calc R . .
C23A C 0.1050(3) 0.7833(2) 0.2125(3) 0.0223(10) Uani 1 1 d . . .
H23A H 0.1062 0.7711 0.2779 0.027 Uiso 1 1 calc R . .
H23B H 0.0948 0.7403 0.1745 0.027 Uiso 1 1 calc R . .
C24A C 0.0141(3) 0.8327(2) 0.1699(3) 0.0235(10) Uani 1 1 d . . .
H24A H 0.0101 0.8427 0.1032 0.028 Uiso 1 1 calc R . .
H24B H -0.0531 0.8110 0.1706 0.028 Uiso 1 1 calc R . .
C25A C 0.0300(3) 0.8993(2) 0.2262(3) 0.0186(10) Uani 1 1 d . . .
H25A H 0.0294 0.8896 0.2918 0.022 Uiso 1 1 calc R . .
H25B H -0.0286 0.9314 0.1972 0.022 Uiso 1 1 calc R . .
C26A C 0.1362(3) 0.9336(2) 0.2282(3) 0.0170(10) Uani 1 1 d . . .
H26A H 0.1344 0.9468 0.1630 0.020 Uiso 1 1 calc R . .
H26B H 0.1463 0.9760 0.2671 0.020 Uiso 1 1 calc R . .
C27A C 0.4860(4) 1.0281(3) 0.1492(3) 0.0167(11) Uani 1 1 d . . .
H27A H 0.5468 1.0547 0.1906 0.020 Uiso 1 1 calc R . .
C28A C 0.5258(4) 0.9870(3) 0.0787(3) 0.0238(12) Uani 1 1 d . . .
H28A H 0.4676 0.9589 0.0382 0.029 Uiso 1 1 calc R . .
H28B H 0.5824 0.9553 0.1135 0.029 Uiso 1 1 calc R . .
C29A C 0.5685(4) 1.0353(3) 0.0159(3) 0.0255(13) Uani 1 1 d . . .
H29A H 0.6306 1.0606 0.0559 0.031 Uiso 1 1 calc R . .
H29B H 0.5916 1.0076 -0.0306 0.031 Uiso 1 1 calc R . .
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C30A C 0.4855(4) 1.0864(3) -0.0360(3) 0.0244(13) Uani 1 1 d . . .
H30A H 0.4266 1.0615 -0.0811 0.029 Uiso 1 1 calc R . .
H30B H 0.5161 1.1187 -0.0727 0.029 Uiso 1 1 calc R . .
C31A C 0.4440(4) 1.1269(3) 0.0335(3) 0.0222(12) Uani 1 1 d . . .
H31A H 0.3864 1.1576 -0.0022 0.027 Uiso 1 1 calc R . .
H31B H 0.5012 1.1562 0.0732 0.027 Uiso 1 1 calc R . .
C32A C 0.4026(4) 1.0794(2) 0.0982(3) 0.0183(11) Uani 1 1 d . . .
H32A H 0.3814 1.1077 0.1453 0.022 Uiso 1 1 calc R . .
H32B H 0.3397 1.0542 0.0596 0.022 Uiso 1 1 calc R . .
Zr2 Zr 0.96872(3) 0.175321(17) 0.39630(3) 0.01100(10) Uani 1 1 d . . .
Cl1B Cl 0.81864(9) 0.16147(6) 0.45721(8) 0.0177(3) Uani 1 1 d . . .
Cl2B Cl 0.99938(9) 0.05790(6) 0.35414(8) 0.0168(3) Uani 1 1 d . . .
Si1B Si 0.99100(11) 0.33935(7) 0.42586(9) 0.0133(3) Uani 1 1 d . . .
Si2B Si 1.15760(10) 0.24174(7) 0.33297(9) 0.0147(3) Uani 1 1 d . . .
C1B C 1.0711(3) 0.2661(2) 0.4928(3) 0.0093(10) Uani 1 1 d . . .
C2B C 1.1429(3) 0.2267(2) 0.4538(3) 0.0125(11) Uani 1 1 d . . .
C3B C 1.1595(3) 0.1627(2) 0.5033(3) 0.0105(10) Uani 1 1 d . . .
H3B H 1.2028 0.1265 0.4928 0.013 Uiso 1 1 calc R . .
C4B C 1.1032(3) 0.1607(3) 0.5692(3) 0.0135(11) Uani 1 1 d . . .
C5B C 1.0488(3) 0.2244(2) 0.5622(3) 0.0129(11) Uani 1 1 d . . .
H5B H 1.0039 0.2370 0.5990 0.015 Uiso 1 1 calc R . .
C6B C 0.9398(3) 0.2850(2) 0.3149(3) 0.0120(10) Uani 1 1 d . . .
C7B C 1.0102(3) 0.2441(2) 0.2757(3) 0.0128(10) Uani 1 1 d . . .
C8B C 0.9468(4) 0.1929(2) 0.2160(3) 0.0133(10) Uani 1 1 d . . .
C9B C 0.8427(4) 0.1996(3) 0.2208(3) 0.0134(10) Uani 1 1 d . . .
H9B H 0.7855 0.1702 0.1903 0.016 Uiso 1 1 calc R . .
C10B C 0.8370(4) 0.2562(2) 0.2773(3) 0.0130(10) Uani 1 1 d . . .
C11B C 0.8912(3) 0.3627(2) 0.4861(3) 0.0171(10) Uani 1 1 d . . .
H11D H 0.9258 0.3864 0.5458 0.026 Uiso 1 1 calc R . .
H11E H 0.8568 0.3207 0.4992 0.026 Uiso 1 1 calc R . .
H11F H 0.8383 0.3933 0.4449 0.026 Uiso 1 1 calc R . .
C12B C 1.0698(3) 0.4175(3) 0.4162(3) 0.0204(11) Uani 1 1 d . . .
H12D H 1.0386 0.4396 0.3546 0.031 Uiso 1 1 calc R . .
H12E H 1.1424 0.4038 0.4218 0.031 Uiso 1 1 calc R . .
H12F H 1.0696 0.4499 0.4670 0.031 Uiso 1 1 calc R . .
C13B C 1.2311(4) 0.3206(3) 0.3137(3) 0.0218(13) Uani 1 1 d . . .
H13D H 1.3013 0.3212 0.3600 0.033 Uiso 1 1 calc R . .
H13E H 1.1923 0.3620 0.3216 0.033 Uiso 1 1 calc R . .
H13F H 1.2380 0.3197 0.2494 0.033 Uiso 1 1 calc R . .
C14B C 1.2262(3) 0.1655(3) 0.3019(3) 0.0202(12) Uani 1 1 d . . .
H14D H 1.2248 0.1686 0.2352 0.030 Uiso 1 1 calc R . .
H14E H 1.1904 0.1231 0.3116 0.030 Uiso 1 1 calc R . .
H14F H 1.2995 0.1646 0.3423 0.030 Uiso 1 1 calc R . .
C15B C 1.1048(4) 0.1030(2) 0.6407(3) 0.0126(10) Uani 1 1 d . . .
H15B H 1.0310 0.0966 0.6432 0.015 Uiso 1 1 calc R . .
C16B C 1.1396(3) 0.03504(17) 0.6063(2) 0.0227(9) Uani 1 1 d . . .
H16D H 1.0972 0.0264 0.5408 0.034 Uiso 1 1 calc R . .
H16E H 1.1298 -0.0028 0.6469 0.034 Uiso 1 1 calc R . .
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H16F H 1.2142 0.0381 0.6093 0.034 Uiso 1 1 calc R . .
C17B C 1.1739(3) 0.1228(2) 0.7423(3) 0.0146(9) Uani 1 1 d . . .
C18B C 1.1292(3) 0.18646(18) 0.7783(2) 0.0236(9) Uani 1 1 d . . .
H18D H 1.1694 0.1953 0.8445 0.035 Uiso 1 1 calc R . .
H18E H 1.0551 0.1783 0.7740 0.035 Uiso 1 1 calc R . .
H18F H 1.1344 0.2265 0.7394 0.035 Uiso 1 1 calc R . .
C19B C 1.1735(3) 0.0632(2) 0.8098(3) 0.0251(10) Uani 1 1 d . . .
H19D H 1.2095 0.0233 0.7928 0.038 Uiso 1 1 calc R . .
H19E H 1.1006 0.0508 0.8049 0.038 Uiso 1 1 calc R . .
H19F H 1.2101 0.0773 0.8749 0.038 Uiso 1 1 calc R . .
C20B C 1.2866(3) 0.13916(19) 0.7437(3) 0.0227(8) Uani 1 1 d . . .
H20D H 1.3273 0.1537 0.8076 0.034 Uiso 1 1 calc R . .
H20E H 1.2860 0.1764 0.6987 0.034 Uiso 1 1 calc R . .
H20F H 1.3190 0.0979 0.7258 0.034 Uiso 1 1 calc R . .
C21B C 0.9819(4) 0.1432(2) 0.1518(3) 0.0138(11) Uani 1 1 d . . .
H21B H 1.0421 0.1155 0.1921 0.017 Uiso 1 1 calc R . .
C22B C 1.0225(4) 0.1842(3) 0.0799(3) 0.0191(11) Uani 1 1 d . . .
H22C H 0.9640 0.2118 0.0386 0.023 Uiso 1 1 calc R . .
H22D H 1.0784 0.2165 0.1144 0.023 Uiso 1 1 calc R . .
C23B C 1.0653(4) 0.1371(3) 0.0199(3) 0.0270(13) Uani 1 1 d . . .
H23C H 1.1274 0.1122 0.0605 0.032 Uiso 1 1 calc R . .
H23D H 1.0883 0.1646 -0.0269 0.032 Uiso 1 1 calc R . .
C24B C 0.9819(4) 0.0853(3) -0.0317(3) 0.0267(13) Uani 1 1 d . . .
H24C H 0.9242 0.1100 -0.0784 0.032 Uiso 1 1 calc R . .
H24D H 1.0135 0.0523 -0.0667 0.032 Uiso 1 1 calc R . .
C25B C 0.9371(4) 0.0459(3) 0.0360(3) 0.0213(12) Uani 1 1 d . . .
H25C H 0.8789 0.0160 -0.0009 0.026 Uiso 1 1 calc R . .
H25D H 0.9925 0.0157 0.0763 0.026 Uiso 1 1 calc R . .
C26B C 0.8962(4) 0.0929(3) 0.0984(3) 0.0175(11) Uani 1 1 d . . .
H26C H 0.8726 0.0650 0.1444 0.021 Uiso 1 1 calc R . .
H26D H 0.8349 0.1191 0.0590 0.021 Uiso 1 1 calc R . .
C27B C 0.7349(3) 0.2875(2) 0.2874(3) 0.0129(10) Uani 1 1 d . . .
H27B H 0.7426 0.2938 0.3564 0.015 Uiso 1 1 calc R . .
C28B C 0.7185(4) 0.3589(2) 0.2390(3) 0.0191(10) Uani 1 1 d . . .
H28C H 0.7802 0.3886 0.2684 0.023 Uiso 1 1 calc R . .
H28D H 0.7129 0.3535 0.1710 0.023 Uiso 1 1 calc R . .
C29B C 0.6186(3) 0.3936(2) 0.2487(3) 0.0269(11) Uani 1 1 d . . .
H29C H 0.6084 0.4385 0.2152 0.032 Uiso 1 1 calc R . .
H29D H 0.6265 0.4025 0.3164 0.032 Uiso 1 1 calc R . .
C30B C 0.5219(3) 0.3476(2) 0.2067(3) 0.0247(11) Uani 1 1 d . . .
H30C H 0.4592 0.3692 0.2182 0.030 Uiso 1 1 calc R . .
H30D H 0.5088 0.3437 0.1373 0.030 Uiso 1 1 calc R . .
C31B C 0.5384(4) 0.2755(3) 0.2512(3) 0.0242(11) Uani 1 1 d . . .
H31C H 0.5415 0.2789 0.3189 0.029 Uiso 1 1 calc R . .
H31D H 0.4775 0.2459 0.2190 0.029 Uiso 1 1 calc R . .
C32B C 0.6376(4) 0.2426(2) 0.2435(3) 0.0170(10) Uani 1 1 d . . .
H32C H 0.6311 0.2344 0.1758 0.020 Uiso 1 1 calc R . .
H32D H 0.6470 0.1973 0.2759 0.020 Uiso 1 1 calc R . .
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C51 C 0.4060(5) 0.7942(4) 0.0937(4) 0.0518(18) Uani 1 1 d . . .
H51A H 0.3824 0.8402 0.0883 0.062 Uiso 1 1 d . . .
H51B H 0.4104 0.7772 0.1573 0.062 Uiso 1 1 d . . .
Cl5 Cl 0.52886(9) 0.78875(6) 0.07809(10) 0.0480(3) Uani 1 1 d . . .
Cl6 Cl 0.30918(11) 0.74423(7) 0.01493(9) 0.0294(3) Uani 1 1 d . . .
C52 C 0.7669(6) 0.8551(4) -0.0427(5) 0.057(2) Uani 0.6464(19) 1 d P . .
H52A H 0.8417 0.8588 -0.0411 0.069 Uiso 0.6464(19) 1 calc PR . .
H52B H 0.7243 0.8803 -0.0994 0.069 Uiso 0.6464(19) 1 calc PR . .
Cl7 Cl 0.7516(2) 0.89424(14) 0.05601(19) 0.0587(8) Uani 0.6464(19) 1 d P .
.
Cl8 Cl 0.73072(19) 0.76883(13) -0.05446(16) 0.0451(7) Uani 0.6464(19) 1 d
P . .
C53 C 0.1013(4) 0.8648(3) 0.9161(4) 0.0346(14) Uani 1 1 d . . .
H53A H 0.1222 0.8429 0.8637 0.041 Uiso 1 1 calc R . .
H53B H 0.0952 0.8280 0.9606 0.041 Uiso 1 1 calc R . .
Cl9 Cl 0.20000(11) 0.92392(7) 0.97580(8) 0.0284(3) Uani 1 1 d . . .
Cl10 Cl -0.02025(9) 0.90465(6) 0.87026(9) 0.0444(3) Uani 1 1 d . . .

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Zr1 0.0106(2) 0.0102(2) 0.0132(2) 0.0003(2) 0.00302(18) 0.0010(2)
Cl1A 0.0156(6) 0.0119(6) 0.0241(6) 0.0010(5) 0.0047(5) -0.0024(5)
Cl2A 0.0129(5) 0.0199(6) 0.0200(5) -0.0014(5) 0.0064(4) 0.0021(5)
Si1A 0.0120(7) 0.0156(8) 0.0124(6) 0.0000(6) 0.0037(5) 0.0013(6)
Si2A 0.0150(7) 0.0103(6) 0.0150(6) -0.0010(5) 0.0043(5) 0.0005(5)
C1A 0.011(2) 0.009(2) 0.017(2) -0.0012(19) -0.0003(19) 0.0035(19)
C2A 0.019(3) 0.013(3) 0.014(2) 0.002(2) 0.0018(19) 0.008(2)
C3A 0.007(2) 0.013(3) 0.017(2) 0.004(2) -0.0004(18) 0.0008(19)
C4A 0.010(2) 0.017(3) 0.009(2) 0.003(2) -0.0017(17) 0.002(2)
C5A 0.009(2) 0.020(3) 0.012(2) 0.008(2) 0.0021(17) 0.003(2)
C6A 0.010(2) 0.015(3) 0.015(2) 0.000(2) 0.0014(19) -0.004(2)
C7A 0.019(3) 0.012(2) 0.011(2) 0.0004(18) 0.0041(19) 0.001(2)
C8A 0.010(2) 0.018(3) 0.011(2) -0.0073(19) -0.0017(18) 0.001(2)
C9A 0.015(2) 0.007(2) 0.012(2) 0.0015(17) -0.0028(18) 0.0004(18)
C10A 0.011(2) 0.012(2) 0.010(2) -0.0029(18) -0.0038(17) -0.0018(19)
C11A 0.020(3) 0.026(3) 0.020(3) -0.002(2) 0.009(2) -0.006(3)
C12A 0.019(3) 0.023(3) 0.018(3) -0.003(2) 0.005(2) 0.008(2)
C13A 0.024(3) 0.016(3) 0.024(2) 0.001(2) 0.003(2) 0.003(2)
C14A 0.021(2) 0.018(2) 0.014(2) 0.0002(17) 0.0045(18) 0.0033(19)
C15A 0.012(2) 0.018(3) 0.018(2) 0.003(2) 0.0011(18) -0.004(2)
C16A 0.017(2) 0.022(2) 0.029(2) -0.0102(17) 0.0106(17) -0.0018(16)
C17A 0.023(2) 0.019(2) 0.013(2) -0.0055(17) 0.0043(17) -0.0006(18)
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C18A 0.018(2) 0.061(3) 0.023(2) -0.013(2) 0.0013(18) -0.005(2)
C19A 0.022(2) 0.025(2) 0.033(3) -0.0118(19) 0.0018(19) 0.0024(19)
C20A 0.047(3) 0.027(2) 0.019(2) -0.0046(19) 0.0003(19) 0.002(2)
C21A 0.018(2) 0.013(2) 0.010(2) 0.0014(16) 0.0046(17) -0.0009(18)
C22A 0.015(2) 0.015(2) 0.023(2) 0.0001(18) 0.0016(18) 0.0026(17)
C23A 0.020(2) 0.013(2) 0.031(3) -0.0042(19) 0.0020(19) -0.0068(17)
C24A 0.017(2) 0.027(2) 0.022(2) 0.0027(19) 0.0003(18) -0.0084(18)
C25A 0.013(2) 0.023(2) 0.016(2) 0.0003(18) -0.0003(17) 0.0012(18)
C26A 0.011(2) 0.019(2) 0.018(2) 0.0005(18) 0.0006(17) -0.0016(18)
C27A 0.015(3) 0.026(3) 0.009(2) 0.000(2) 0.003(2) 0.000(2)
C28A 0.028(3) 0.017(3) 0.027(3) 0.001(2) 0.010(2) 0.009(3)
C29A 0.027(3) 0.034(3) 0.020(3) 0.006(2) 0.014(2) -0.001(3)
C30A 0.033(3) 0.026(3) 0.015(2) 0.012(2) 0.008(2) -0.004(2)
C31A 0.026(3) 0.019(3) 0.019(2) 0.008(2) 0.003(2) -0.009(2)
C32A 0.017(3) 0.016(3) 0.018(2) 0.003(2) -0.002(2) 0.000(2)
Zr2 0.0112(2) 0.0103(2) 0.0115(2) -0.00060(19) 0.00340(18) -0.0011(2)
Cl1B 0.0164(6) 0.0194(6) 0.0192(5) -0.0002(5) 0.0083(4) -0.0018(5)
Cl2B 0.0179(6) 0.0130(6) 0.0191(6) -0.0031(5) 0.0045(5) -0.0016(5)
Si1B 0.0154(7) 0.0100(6) 0.0124(6) 0.0002(5) 0.0008(5) -0.0004(5)
Si2B 0.0114(7) 0.0164(8) 0.0154(7) 0.0027(6) 0.0025(5) -0.0016(6)
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C9B 0.011(2) 0.019(3) 0.010(2) 0.0025(18) 0.0033(18) -0.0019(19)
C10B 0.020(3) 0.009(2) 0.009(2) 0.0017(17) 0.0028(19) 0.001(2)
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C12B 0.020(3) 0.013(2) 0.027(2) 0.004(2) 0.005(2) 0.002(2)
C13B 0.020(3) 0.026(3) 0.020(3) 0.001(2) 0.007(2) -0.007(2)
C14B 0.013(3) 0.028(3) 0.018(2) 0.001(2) 0.002(2) 0.000(2)
C15B 0.018(2) 0.007(2) 0.016(2) 0.0055(18) 0.0104(18) -0.0011(19)
C16B 0.032(2) 0.0160(18) 0.017(2) 0.0002(15) 0.0031(17) -0.0010(16)
C17B 0.018(2) 0.015(2) 0.011(2) 0.0024(16) 0.0053(16) -0.0001(17)
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C19B 0.030(2) 0.022(2) 0.022(2) 0.0095(18) 0.0063(19) 0.0059(19)
C20B 0.020(2) 0.028(2) 0.017(2) 0.0046(17) 0.0010(16) -0.0022(17)
C21B 0.013(2) 0.012(2) 0.016(2) -0.0032(19) 0.0033(19) 0.001(2)
C22B 0.020(3) 0.029(3) 0.011(2) -0.004(2) 0.007(2) 0.003(2)
C23B 0.031(3) 0.033(3) 0.020(3) -0.003(2) 0.010(2) 0.000(3)
C24B 0.028(3) 0.030(3) 0.023(3) -0.004(2) 0.009(2) 0.010(3)
C25B 0.022(3) 0.023(3) 0.016(2) -0.003(2) 0.001(2) 0.000(2)
C26B 0.020(3) 0.019(3) 0.016(2) -0.002(2) 0.008(2) 0.005(2)
C27B 0.010(2) 0.014(2) 0.012(2) -0.0021(17) -0.0012(16) 0.0019(18)
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C31B 0.011(2) 0.037(3) 0.022(2) 0.000(2) 0.0018(18) -0.0005(19)
C32B 0.019(2) 0.013(2) 0.020(2) 0.0014(18) 0.0074(19) 0.0008(18)
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Cl6 0.0316(7) 0.0266(7) 0.0284(7) -0.0048(6) 0.0063(6) -0.0034(6)
C52 0.051(5) 0.062(5) 0.049(5) 0.021(4) 0.001(4) -0.026(4)
Cl7 0.0491(15) 0.0461(16) 0.0911(19) -0.0013(14) 0.0363(14) 0.0104(11)
Cl8 0.0466(14) 0.0433(14) 0.0461(13) 0.0113(11) 0.0150(10) 0.0137(11)
C53 0.024(3) 0.026(3) 0.049(3) -0.025(3) 0.004(2) -0.002(2)
Cl9 0.0393(8) 0.0207(7) 0.0218(6) -0.0025(5) 0.0037(5) -0.0072(6)
Cl10 0.0343(7) 0.0344(6) 0.0549(8) -0.0136(6) -0.0017(6) 0.0080(5)

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;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Zr1 C12A 2.4322(12) . yes
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Zr1 C3A 2.532(4) . yes
Zr1 C5A 2.539(4) . yes
Zr1 C10A 2.612(4) . yes
Zr1 C8A 2.612(4) . yes
Zr1 C9A 2.645(4) . yes
Zr1 C4A 2.646(4) . yes
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Si1A C11A 1.855(5) . ?
Si1A C1A 1.880(5) . ?
Si1A C6A 1.885(4) . ?
Si2A C14A 1.865(5) . ?
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Zr2 C10B 2.605(4) . yes
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